

# Solution of the Skyrme-Hartree-Fock equations in the Cartesian deformed harmonic oscillator basis. (I) The method.

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## Abstract

We describe a method of solving the nuclear Skyrme-Hartree-Fock problem by using a deformed Cartesian harmonic oscillator basis. The complete list of expressions required to calculate local densities, total energy, and self-consistent fields is presented, and an implementation of the self-consistent symmetries is discussed. Formulas to calculate matrix elements in the Cartesian harmonic oscillator basis are derived for the nuclear and Coulomb interactions.

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## 1 Introduction

Self-consistent methods have been used in the low-energy nuclear structure studies over many years, and represent a mature field with numerous successful applications, see Refs. [1, 2, 3, 4, 5] for a review. A number of computer codes solving the nuclear Hartree-Fock (HF) problem have already been developed. Two types of effective nucleon-nucleon interactions have been mainly employed. Starting with the work of Vautherin and Brink [6] many authors have applied the nuclear HF theory with the Skyrme effective interaction, while the work of Gogny [7, 8] initiated numerous studies with the force which carries his name.

The methods employed to solve the HF equations depend mainly on the effective force used and on the assumed symmetries of the many-body wave functions. For the solutions which allow at least triaxial deformations, two different methods have been applied for the two abovementioned effective interactions. The first one, used in conjunction with the Skyrme interaction, is formulated in the spatial coordinates and makes use of the finite-difference [9], or Fourier [10], or spline-collocation [11, 12] methods to approximate differential operators. The solution is then obtained by using the imaginary time evolution operator [13].

The second one, used for the finite-range Gogny interaction, employs a truncated harmonic oscillator (HO) basis [14, 15] and solves the problem either by an iterative

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diagonalization of the mean-field Hamiltonian, or by the gradient- [16] or the conjugate gradient- [17] methods. A similar basis-expansion technique has also been recently used [18] for studies in the frame of the relativistic mean field theory, for a review cf. Ref. [19]. The present study aims at describing the method which incorporates the advantages of both existing approaches, and combines the robustness of the Cartesian HO basis with the simplicity of the Skyrme interaction.

The methods using spatial coordinates have several advantages. First of all, various nuclear shapes can be easily treated on the same footing; the same cubic lattice of points in three spatial dimensions is suitable to accommodate wave functions with, in principle, arbitrary deformations restricted only by a specific symmetrization of the lattice. This allows easy studies of systems for which the deformation is not *a priori* known, or is ill defined because of deformation instabilities or a shape coexistence. Secondly, using spatial coordinates allows studies which address the asymptotic form of nucleonic wave functions at large distances. This is particularly important for a precise description of weakly bound nuclei, where the use of spatial coordinates is a necessity [20]. Third, for the Skyrme zero-range interaction, the mean fields are local (apart from a velocity dependence) and can be easily programmed in the spatial coordinates. Last but not least, the treatment of wave functions on large lattices ( $12 \times 12 \times 12$  is a typical example) is easily amenable to vectorization or parallelization of the algorithm.

Methods using the HO basis have other advantages. Firstly, the basis provides a natural cut-off for many operators which otherwise are unbound and require particularly delicate treatment in the spatial coordinates. This concerns in particular the multipole moment and the angular momentum operators which are often used as constraining operators. For the corresponding constraints the solutions can become unstable when the non-zero probability amplitudes (wave functions) move towards large distances as it is the case for e.g. weakly bound nucleons. Secondly, much smaller spaces are usually required to describe the nuclear wave functions within a given precision. Typically a basis of about 300 HO wave functions is sufficient for most applications. Third, the iterative diagonalization of the mean field Hamiltonian can be used to find the self-consistent solutions, which provides a rapidly converging algorithm, and, last but not least, scalar or super scalar computers can also be used, because the typical sizes of the information handled is smaller and the performance is less dependent on the use of a vector processor.

The above listed advantages of a given method correspond often (although not always) to the disadvantages of the other one, and both methods described above are in this respect complementary. Our motivation to construct the Skyrme-Hartree-Fock code using the Cartesian HO basis was based on the necessity to obtain a tool which would allow rapid solutions for the nuclear superdeformed or hyperdeformed rotating states for which the deformation is relatively well known *a priori*. Indeed, the method employed by us gives a particularly fast, stable, robust, and simple algorithm to solve such physical problems.

The paper is organized in the following way. In Sec. 2 we present the HF method for the Skyrme interaction, and in particular we discuss the local densities, total energy, constraints, mean fields, and HF equations. In Sec. 3 we describe the use of various symmetries and in Sec. 4 the use of the Cartesian HO basis. Sec. 5 is devoted to the new method we use to calculate the direct Coulomb potential. The method described in the present study is implemented in the computer code HFODD, published in the subsequent

paper [21] which is referred to as II.

## 2 Hartree-Fock method

In this Section we present the complete set of formulas which are used when solving the Skyrme-Hartree-Fock problem.

### 2.1 Local densities

In the HF approximation, the total energy of a nuclear system is, in general, a functional of the one-body non-local density defined as

$$\rho_\alpha(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \langle \Psi | a_{\mathbf{r}'\sigma'\alpha}^\dagger a_{\mathbf{r}\sigma\alpha} | \Psi \rangle. \quad (1)$$

Here,  $|\Psi\rangle$  is a many-body wave function, and  $a_{\mathbf{r}\sigma\alpha}^\dagger$  and  $a_{\mathbf{r}\sigma\alpha}$  are the operators creating and annihilating a neutron ( $\alpha=n$ ) or a proton ( $\alpha=p$ ) in the space-point  $\mathbf{r}$  and having the projection of spin  $\sigma=\pm\frac{1}{2}$ .

The non-local density (1) can be written [22] as a sum of the scalar,  $\rho_\alpha(\mathbf{r}, \mathbf{r}')$ , and vector,  $\mathbf{s}_\alpha(\mathbf{r}, \mathbf{r}')$  terms, defined by

$$\rho_\alpha(\mathbf{r}, \mathbf{r}') = \sum_\sigma \rho_\alpha(\mathbf{r}\sigma, \mathbf{r}'\sigma) \quad (2)$$

and

$$\mathbf{s}_\alpha(\mathbf{r}, \mathbf{r}') = \sum_{\sigma\sigma'} \rho_\alpha(\mathbf{r}\sigma, \mathbf{r}'\sigma') < \sigma' | \boldsymbol{\sigma} | \sigma > \quad (3)$$

as

$$\rho_\alpha(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \frac{1}{2} \rho_\alpha(\mathbf{r}, \mathbf{r}') \delta_{\sigma\sigma'} + \frac{1}{2} \mathbf{s}_\alpha(\mathbf{r}, \mathbf{r}') \cdot \boldsymbol{\sigma}_{\sigma\sigma'}. \quad (4)$$

Assuming that the total energy depends only on local ( $\mathbf{r}=\mathbf{r}'$ ) densities, and on their derivatives at  $\mathbf{r}=\mathbf{r}'$  up to the second order, one has to consider the following real nucleonic densities [22]:

- particle-density  $\rho_\alpha(\mathbf{r})$  and spin density  $\mathbf{s}_\alpha(\mathbf{r})$ ,

$$\rho_\alpha(\mathbf{r}) = \rho_\alpha(\mathbf{r}, \mathbf{r}), \quad (5a)$$

$$\mathbf{s}_\alpha(\mathbf{r}) = \mathbf{s}_\alpha(\mathbf{r}, \mathbf{r}), \quad (5b)$$

- kinetic density  $\tau_\alpha(\mathbf{r})$  and vector kinetic density  $\mathbf{T}_\alpha(\mathbf{r})$ ,

$$\tau_\alpha(\mathbf{r}) = [\nabla \cdot \nabla' \rho_\alpha(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (6a)$$

$$\mathbf{T}_\alpha(\mathbf{r}) = [\nabla \cdot \nabla' \mathbf{s}_\alpha(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (6b)$$

- momentum density  $\mathbf{j}_\alpha(\mathbf{r})$  and spin-current tensor  $\overleftrightarrow{J}_\alpha(\mathbf{r})$ ,

$$\mathbf{j}_\alpha(\mathbf{r}) = \frac{1}{2i} [(\nabla - \nabla') \rho_\alpha(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (7a)$$

$$J_{\mu\nu,\alpha}(\mathbf{r}) = \frac{1}{2i} [(\nabla_\mu - \nabla'_\mu) s_{\nu,\alpha}(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}. \quad (7b)$$

In what follows we often omit the space argument  $\mathbf{r}$  of local densities.

For each of the local densities we define the isoscalar and isovector density. For example, the isoscalar ( $\rho_0$ ) and isovector ( $\rho_1$ ) particle densities are defined as

$$\rho_0 = \rho_n + \rho_p, \quad \rho_1 = \rho_n - \rho_p. \quad (8)$$

Following a traditional notation, for isoscalar densities we sometimes omit the isospin index, for example,  $\rho \equiv \rho_0$ .

## 2.2 Hartree-Fock energy

In the Skyrme-HF approximation, the total energy  $\mathcal{E}$  of a nucleus is given as a sum of the kinetic, Skyrme, Coulomb, and pairing terms

$$\mathcal{E} = \mathcal{E}^{\text{kin}} + \mathcal{E}^{\text{Skyrme}} + \mathcal{E}^{\text{Coul}} + \mathcal{E}^{\text{pair}}. \quad (9)$$

The kinetic energy of both protons and neutrons is given by the integral of the isoscalar kinetic density  $\tau_0(\mathbf{r})$ , cf. Eqs. (6a) and (8),

$$\mathcal{E}^{\text{kin}} = \frac{\hbar^2}{2m} \left(1 - \frac{1}{A}\right) \int d^3\mathbf{r} \tau_0(\mathbf{r}), \quad (10)$$

where the standard factor  $(1 - \frac{1}{A})$  provides a simple approximation to the center-of-mass correction [23] in terms of the number of nucleons  $A$ .

The Skyrme energy is the sum of the isoscalar ( $t=0$ ) and isovector ( $t=1$ ) terms, and is given as the integral of two energy densities. The first of these densities,  $\mathcal{H}_t^{\text{even}}(\mathbf{r})$ , depends on the time-even densities  $\rho_t$ ,  $\tau_t$ , and  $\vec{J}_t \equiv J_{\mu\nu,t}$ , while the second one,  $\mathcal{H}_t^{\text{odd}}(\mathbf{r})$ , depends on the time-odd densities,  $\mathbf{s}_t$ ,  $\mathbf{T}_t$ ,  $\mathbf{j}_t$  (see Ref. [24]), i.e.,

$$\mathcal{E}^{\text{Skyrme}} = \sum_{t=0,1} \int d^3\mathbf{r} \left( \mathcal{H}_t^{\text{even}}(\mathbf{r}) + \mathcal{H}_t^{\text{odd}}(\mathbf{r}) \right), \quad (11)$$

for

$$\mathcal{H}_t^{\text{even}}(\mathbf{r}) \equiv C_t^\rho \rho_t^2 + C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^\tau \rho_t \tau_t + C_t^J \vec{J}_t^{\leftrightarrow 2} + C_t^{\nabla J} \rho_t \nabla \cdot \mathbf{J}_t, \quad (12a)$$

$$\mathcal{H}_t^{\text{odd}}(\mathbf{r}) \equiv C_t^s \mathbf{s}_t^2 + C_t^{\Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t + C_t^T \mathbf{s}_t \cdot \mathbf{T}_t + C_t^j \mathbf{j}_t^2 + C_t^{\nabla j} \mathbf{s}_t \cdot (\nabla \times \mathbf{j}_t). \quad (12b)$$

In Eq. (12a), the square of the tensor density is defined as  $\vec{J}_t^{\leftrightarrow 2} \equiv \sum_{\mu\nu} J_{\mu\nu,t}^2$ , and its vector part  $\mathbf{J}_t$  is defined as  $J_{\lambda,t} \equiv \sum_{\mu\nu} \epsilon_{\lambda\mu\nu} J_{\mu\nu,t}$ .

Expressions introduced via Eqs. (12), relating the ten time-even coupling constants  $C_t^\rho$ ,  $C_t^{\Delta\rho}$ ,  $C_t^\tau$ ,  $C_t^J$ , and  $C_t^{\nabla J}$ , and the ten time-odd coupling constants  $C_t^s$ ,  $C_t^{\Delta s}$ ,  $C_t^T$ ,  $C_t^j$ , and  $C_t^{\nabla j}$ , to the standard parameters of the Skyrme interaction are given in Ref. [24]. Internally, the code HFODD uses the coupling constants in the traditional representation in which every term is a sum of the total density squared, and of the sum of squares of neutron and proton densities. Every such a term can also be written down in the isoscalar-isovector representation used in Eqs. (11) and (12). For the simplest term depending on particle densities, the correspondence is

$$C_{\text{tot}}^\rho (\rho_n + \rho_p)^2 + C_{\text{sum}}^\rho (\rho_n^2 + \rho_p^2) = C_0^\rho (\rho_n + \rho_p)^2 + C_1^\rho (\rho_n - \rho_p)^2, \quad (13)$$

which trivially leads to the following relations between both sets of the coupling constants

$$C_{\text{tot}}^\rho = C_0^\rho - C_1^\rho, \quad (14a)$$

$$C_{\text{sum}}^\rho = 2C_1^\rho, \quad (14b)$$

or equivalently

$$C_0^\rho = \frac{1}{2}C_{\text{sum}}^\rho + C_{\text{tot}}^\rho, \quad (15a)$$

$$C_1^\rho = \frac{1}{2}C_{\text{sum}}^\rho. \quad (15b)$$

Analogous relations hold for all other terms in the energy density.

The Coulomb energy is a sum of the direct and exchange contributions,

$$\mathcal{E}^{\text{Coul}} = \mathcal{E}_{\text{dir}}^{\text{Coul}} + \mathcal{E}_{\text{exch}}^{\text{Coul}}, \quad (16)$$

for

$$\mathcal{E}_{\text{dir}}^{\text{Coul}} = \frac{e^2}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\rho_p(\mathbf{r}_1)\rho_p(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (17a)$$

$$\mathcal{E}_{\text{exch}}^{\text{Coul}} = \frac{e^2}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\rho_p(\mathbf{r}_2, \mathbf{r}_1)\rho_p(\mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (17b)$$

where  $\rho_p(\mathbf{r})$  and  $\rho_p(\mathbf{r}_1, \mathbf{r}_2)$  are the local and non-local proton densities, respectively, Eqs. (5a) and (2), and  $e$  is the elementary charge. By using expressions (17) we approximate the charge density by the proton density without taking into account neither proton and neutron charge form factors [25] nor other corrections [26] which turn out to be small.

In the algorithm, the direct Coulomb energy is calculated as the trace of the proton density matrix with the HO matrix elements of the Coulomb potential (see Sec. 5). The Coulomb energy  $U^{\text{Coul}}(\mathbf{r})$  is given by

$$U^{\text{Coul}}(\mathbf{r}) = e^2 \int d\mathbf{r}' \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (18)$$

where, in order to express  $U^{\text{Coul}}(\mathbf{r})$  in units of energy, the additional factor  $e$  is added as compared to the standard electrostatic expression.

The exchange Coulomb energy is calculated in the Slater approximation [27, 28]:

$$\mathcal{E}_{\text{exch}}^{\text{Coul}} = -\frac{3e^2}{4} \left(\frac{3}{\pi}\right)^{1/3} \int d\mathbf{r} \rho_p^{4/3}(\mathbf{r}). \quad (19)$$

The term  $\mathcal{E}^{\text{pair}}$  is equal to the average value of the seniority pairing interaction [1] calculated in the BCS state:

$$\mathcal{E}^{\text{pair}} = - \sum_{\alpha=n,p} \frac{G_\alpha}{4} \left( \sum_i u_{i,\alpha} v_{i,\alpha} \right)^2, \quad (20)$$

where  $G_n$  and  $G_p$  are the neutron and proton pairing strengths, respectively, taken from Ref. [29]. Sums are performed separately over the neutron and proton single-particle states, while the standard BCS occupation factors,  $v_{i,\alpha}$  satisfy as always  $v_{i,\alpha}^2 + u_{i,\alpha}^2 = 1$ . Note that  $\mathcal{E}^{\text{pair}}$  does not correspond to the difference between the energies of unpaired and paired solutions, because the occupation factors also influence other terms in the total energy. In the present version of the code HFODD the pairing correlations are included only within the non-rotating case, see II.

### 2.3 Constraints

The total energy (9) can be minimized under specific constraints. One of the most essential ones is related to the so-called cranking approximation which is equivalent to solving the time-dependent HF equations in the laboratory frame or the HF equations in the rotating frame [1]. To distinguish between the energy operators and/or eigenvalues written either in the laboratory frame or in the turning reference frame, the latter ones are referred to as Routhians. This notion applies also to situations when other constraints are taken into account.

In order to find a constrained minimum of energy one has to find a minimum of the Routhian  $\mathcal{E}'$  defined by

$$\mathcal{E}' = \mathcal{E} + \mathcal{E}^{\text{mult}} + \mathcal{E}^{\text{cran}} + \mathcal{E}^{\text{numb}}, \quad (21)$$

i.e., equal to the sum of the energy and the terms responsible for the multipole, cranking, and particle-number constraints, respectively, as defined below.

The multipole constraints are assumed in the standard quadratic form [30]:

$$\mathcal{E}^{\text{mult}} = \sum_{\lambda\mu} C_{\lambda\mu} \left( \langle \hat{Q}_{\lambda\mu} \rangle - \bar{Q}_{\lambda\mu} \right)^2, \quad (22)$$

where  $\langle \hat{Q}_{\lambda\mu} \rangle$  are the average values of the mass-multipole-moment operators,  $\bar{Q}_{\lambda\mu}$  are the constraint values of the multipole moments, and  $C_{\lambda\mu}$  are the stiffness constants.

The cranking constraints aim at finding solutions corresponding to non-zero angular momenta, and are assumed in a combined form of the linear and quadratic constraints:

$$\mathcal{E}^{\text{cran}} = -\omega_J \langle \hat{J}_y \rangle + C_J \left( \langle \hat{J}_y \rangle - \bar{J}_y \right)^2, \quad (23)$$

where  $\hat{J}_y$  is the operator of the component of the total angular momentum along the  $y$  axis, and  $\bar{J}_y$  is the corresponding target value. The code HFODD uses the  $y$  axis as the cranking axis and assumes that the  $x$ - $z$  plane as the conserved symmetry plane (see below for more details). For the combined constraint, the physical angular frequency  $\omega$  is given by

$$\omega_y = \frac{\partial \mathcal{E}}{\partial \langle \hat{J}_y \rangle} = \omega_J - 2C_J \left( \langle \hat{J}_y \rangle - \bar{J}_y \right), \quad (24)$$

It turns out that a pure linear constraint ( $C_J=0$ ) leads to a much more stable convergence properties, and then  $\omega_y = \omega_J$ .

The particle-number constraints ensure the correct average values of neutron and proton numbers when the pairing option is used, and are assumed in the standard linear forms, i.e.,

$$\mathcal{E}^{\text{numb}} = -\lambda_n \langle \hat{N}_n \rangle - \lambda_p \langle \hat{N}_p \rangle, \quad (25)$$

where  $\lambda_n$  and  $\lambda_p$  are the neutron and proton Fermi energies, and  $\hat{N}_n$  and  $\hat{N}_p$  are the corresponding neutron and proton particle-number operators. The particle number constraints are taken into account only when the pairing correlations are included (in the non-rotating case, at present). Otherwise the numbers of particles are defined by selecting a given number of occupied states explicitly (see II, Sec. 3.4).

## 2.4 Hartree-Fock mean fields

Upon a variation of the total Routhian (21) with respect to neutron and proton single-particle wave functions, one obtains the HF single-particle Routhian operators in the form:

$$h'_n = -\frac{\hbar^2}{2m}\Delta + \left(\Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} + \Gamma_1^{\text{even}} + \Gamma_1^{\text{odd}}\right) + U^{\text{mult}} - \omega_y \hat{J}_y, \quad (26a)$$

$$h'_p = -\frac{\hbar^2}{2m}\Delta + \left(\Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} - \Gamma_1^{\text{even}} - \Gamma_1^{\text{odd}}\right) + U^{\text{Coul}} + U^{\text{mult}} - \omega_y \hat{J}_y. \quad (26b)$$

The momentum dependent potentials  $\Gamma$  are given by [22, 24]

$$\Gamma_t^{\text{even}} = -\nabla \cdot [M_t(\mathbf{r})\nabla] + U_t(\mathbf{r}) + \frac{1}{2i} \left( \vec{\nabla}\sigma \cdot \vec{B}_t(\mathbf{r}) + \vec{B}_t(\mathbf{r}) \cdot \vec{\nabla}\sigma \right), \quad (27a)$$

$$\Gamma_t^{\text{odd}} = -\nabla \cdot \left[ (\boldsymbol{\sigma} \cdot \mathbf{C}_t(\mathbf{r}))\nabla \right] + \boldsymbol{\sigma} \cdot \boldsymbol{\Sigma}_t(\mathbf{r}) + \frac{1}{2i} \left( \nabla \cdot \mathbf{I}_t(\mathbf{r}) + \mathbf{I}_t(\mathbf{r}) \cdot \nabla \right). \quad (27b)$$

In Eqs. (26),  $U^{\text{mult}}$  represents the terms originating from the multipole constraints:

$$U^{\text{mult}} = 2 \sum_{\lambda\mu} C_{\lambda\mu} \left( \langle \hat{Q}_{\lambda\mu} \rangle - \bar{Q}_{\lambda\mu} \right) \hat{Q}_{\lambda\mu}. \quad (28)$$

With pairing correlations taken into account, the single-particle Routhians should in principle also contain the terms  $-\lambda_\alpha \hat{N}_\alpha$  originating from the particle number constraint (25). However, usually these terms are kept aside and included in the equations explicitly. Such a convention allows keeping for the single-particle Routhians the convenient standard energy scale.

The functions defining the HF potentials (27) depend on the local densities (5)–(7), and read [24]

$$U_t = 2C_t^\rho \rho_t + 2C_t^{\Delta\rho} \Delta\rho_t + C_t^\tau \tau_t + C_t^{\nabla J} \nabla \cdot \mathbf{J}_t + U'_t, \quad (29a)$$

$$\boldsymbol{\Sigma}_t = 2C_t^s \mathbf{s}_t + 2C_t^{\Delta s} \Delta \mathbf{s}_t + C_t^T \mathbf{T}_t + C_t^{\nabla j} \nabla \times \mathbf{j}_t, \quad (29b)$$

$$M_t = C_t^\tau \rho_t, \quad (29c)$$

$$\mathbf{C}_t = C_t^T \mathbf{s}_t, \quad (29d)$$

$$\vec{B}_t = 2C_t^J \vec{J}_t - C_t^{\nabla J} \vec{\nabla} \rho_t, \quad (29e)$$

$$\mathbf{I}_t = 2C_t^j \mathbf{j}_t + C_t^{\nabla j} \nabla \times \mathbf{s}_t. \quad (29f)$$

The tensor gradient operators in Eqs. (27) and (29e) are defined [22] as  $(\vec{\nabla}\sigma)_{\mu\nu} = \nabla_\mu \sigma_\nu$  and  $\nabla_{\mu\nu} = \sum_\lambda \epsilon_{\mu\nu\lambda} \nabla_\lambda$ .

In Eq. (29a) the term  $U'_t$  represents the rearrangement terms resulting from the density dependence of the coupling constants. In standard parametrizations of the Skyrme forces, which are implemented in the code HFODD, only the  $C_t^\rho$  and  $C_t^s$  coupling constants depend on the isoscalar density  $\rho_0$ , and then

$$U'_t = \delta_{t0} \sum_{t'=0,1} \left( \frac{\partial C_{t'}^\rho}{\partial \rho_0} \rho_{t'}^2 + \frac{\partial C_{t'}^s}{\partial \rho_0} s_{t'}^2 \right). \quad (30)$$

## 2.5 Hartree-Fock equations

The eigenequations for the HF single-particle Routhians (26) are called HF equations, and read

$$h'_\alpha \psi_{i,\alpha}(\mathbf{r}\sigma) = e'_{i,\alpha} \psi_{i,\alpha}(\mathbf{r}\sigma). \quad (31)$$

The single-particle index  $i$  comprises all nucleonic quantum numbers. We use the convention that this index has different values for both members within the time-reversed, or signature-reversed, or simplex-reversed couples (see Sec. 3), i.e., every single-particle state is considered separately, and the sums over  $i$  are performed over *all* neutron or proton single-particle states. This is in contrast to some formulations where the sums are performed over only one-half of states which have one common value of, e.g., the signature, or one sign of the spin projection. [Note, for example, the factor  $\frac{1}{4}$  in Eq. (20).]

The standard way of assessing the quality of convergence of the HF equations is to compare the value of energy  $\mathcal{E}$  calculated from Eqs. (9)–(20) with that calculated by using the sum of the single-particle energies

$$\mathcal{E}^{\text{s.p.}} = \sum_{i,\alpha} v_{i,\alpha}^2 e_{i,\alpha}. \quad (32)$$

A connection between these two energies exists because  $\mathcal{E}^{\text{s.p.}}$  is related to the average value of the single-particle Routhian, which for a density independent interaction and with no constraints is trivially equal to the average kinetic energy plus twice the average two-body interaction energy [1]. In the realistic case of the density-dependent interactions, this simple relation has to be modified and one defines the equivalent energy  $\tilde{\mathcal{E}}$  by

$$\tilde{\mathcal{E}} = \frac{1}{2} \mathcal{E}^{\text{s.p.}} + \frac{1}{2} \mathcal{E}^{\text{kin}} + \mathcal{E}^{\text{pair}} - \mathcal{E}^{\text{rear}} + \frac{1}{3} \mathcal{E}_{\text{exch}}^{\text{Coul}} - \mathcal{E}_{\text{corr}}^{\text{mult}} - \mathcal{E}_{\text{corr}}^{\text{cran}} \quad (33)$$

Here, the rearrangement energy  $\mathcal{E}^{\text{rear}}$  results from the density dependence of the Skyrme interaction and is equal to one half of the average value of rearrangement potential Eq. (30),

$$\mathcal{E}^{\text{rear}} = \frac{1}{2} \int d^3\mathbf{r} U'_0 \rho_0. \quad (34)$$

Similarly, the Coulomb exchange energy (19) can be considered as resulting from a zero-order interaction term depending on the density as  $\rho_p^{-2/3}$ . Hence the resulting rearrangement term in Eq. (33) is equal to the Coulomb exchange energy with the factor  $\frac{1}{3}$ . Finally, the corrections resulting from the constraints read

$$\mathcal{E}_{\text{corr}}^{\text{mult}} = \sum_{\lambda\mu} C_{\lambda\mu} \left( \langle \hat{Q}_{\lambda\mu} \rangle - \bar{Q}_{\lambda\mu} \right) \langle \hat{Q}_{\lambda\mu} \rangle \quad (35)$$



for the multipole constraints (28), and

$$\mathcal{E}_{\text{corr}}^{\text{cran}} = -\frac{1}{2}\omega_y \langle \hat{J}_y \rangle \quad (36)$$

for the cranking constraint with  $\omega_y$  given by Eq. (24). Since the term corresponding to the particle number constraint is not included in the Routhian, the correction for this constraint does not appear in  $\tilde{\mathcal{E}}$ .

The difference between the energies  $\tilde{\mathcal{E}}$  and  $\mathcal{E}$  is exactly equal to zero when the densities and fields do not change from one iteration to the next one. Hence their difference

$$\delta\mathcal{E} = \tilde{\mathcal{E}} - \mathcal{E} \quad (37)$$

provides a useful measure of the quality of convergence, and is called the stability of the HF energy. In practice,  $\mathcal{E}$  approaches faster the final value of the total energy than does  $\tilde{\mathcal{E}}$ .

## 2.6 Hartree-Fock densities

In terms of the Routhian eigenfunctions, the non-local density matrix is given by

$$\rho_\alpha(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \sum_i v_{i,\alpha}^2 \psi_{i,\alpha}(\mathbf{r}\sigma) \psi_{i,\alpha}^*(\mathbf{r}'\sigma'). \quad (38)$$

The occupation factors  $v_{i,\alpha}^2$  are determined through the standard BCS procedure (when the pairing correlations are taken into account for the non-rotating case of the code HFODD), or are equal to 1 or 0 according to the chosen configuration (when the pairing correlations are not used).

The energy densities (12) depend on the six real densities  $\rho_t$ ,  $\tau_t$ ,  $\mathbf{s}_t$ ,  $\mathbf{T}_t$ ,  $\mathbf{j}_t$ , and  $\overleftrightarrow{\mathbf{j}}_t$ . Each of them has the isoscalar ( $t=0$ ) and isovector ( $t=1$ ) form, or equivalently, the neutron and proton form. Moreover, in Eqs. (12) and (29) there also appear six secondary densities which are some particular derivatives of the six basic ones, i.e.,  $\Delta\rho_t$ ,  $\nabla \cdot \mathbf{J}_t$ ,  $\Delta\mathbf{s}_t$ ,  $\nabla\rho_t$ ,  $\nabla \times \mathbf{j}_t$ , and  $\nabla \times \mathbf{s}_t$ . In principle, they can be calculated by an explicit numerical derivation of the six basic densities. However, the organization of the code HFODD allows calculating them directly at a negligible expense of the CPU time. This is so, because the principal numerical effort must anyhow be devoted to summing up the contributions of the HO basis states to the HF eigenstates at every point in space (see Sec. 4.2). Once this is accomplished, the remaining operations are very rapid.

The scheme used in the code HFODD is therefore the following. First, at every point of space,  $\mathbf{r}$ , and for every spin value  $\sigma$ , the values of the HF wave functions, their derivatives in three directions, and their Laplacians are calculated. At this point it is convenient to combine the value of each wave function and its three derivatives into one four-vector. To this effect we introduce the symbolic notation for derivatives,  $\nabla_{\hat{\mu}}$ , which are distinguished by hatted indices taking values  $\hat{\mu}=0, 1, 2, 4$ . Then,  $\hat{\mu}=0$  corresponds to the unity operator (no derivative involved), and the three usual indices correspond to the usual gradient in space, i.e.,  $\nabla_{\hat{\mu}} \equiv (1, \nabla)$ . By using this notation we define the two following generic matrices of densities:

$$D_{\hat{\mu}\hat{\nu},\alpha}^{qq'} = \sum_i v_{i,\alpha}^2 [\nabla_{\hat{\mu}} \psi_{i,\alpha}(\mathbf{r}\sigma)] [\nabla_{\hat{\nu}} \psi_{i,\alpha}^*(\mathbf{r}\sigma')], \quad (39a)$$

$$L_{\alpha}^{qq'} = \sum_i v_{i,\alpha}^2 \psi_{i,\alpha}(\mathbf{r}\sigma) \Delta \psi_{i,\alpha}^*(\mathbf{r}\sigma'), \quad (39b)$$

where indices  $q$  and  $q'$  denote the signs of spin variables  $\sigma$  and  $\sigma'$ , respectively, i.e.,  $q=+$  for  $\sigma=+\frac{1}{2}$  and  $q=-$  for  $\sigma=-\frac{1}{2}$ .

The local densities required for the calculation of energies and fields have to be determined separately for neutrons and protons. Below we omit for simplicity the isospin indices and denote by  $\Re$  and  $\Im$  the real and imaginary parts. Then the required 34 real densities are given in terms of 64 complex or real densities  $D_{\mu\nu}^{qq'}$  and 4 complex densities  $L^{qq'}$  by the following expressions:

- scalar densities

$$\rho = D_{00}^{++} + D_{00}^{--}, \quad (40)$$

$$\tau = \sum_{\mu} (D_{\mu\mu}^{++} + D_{\mu\mu}^{--}), \quad (41)$$

$$\Delta\rho = 2\Re(L^{++} + L^{--}) + 2\tau, \quad (42)$$

$$\nabla \cdot \mathbf{J} = -2\Im(D_{23}^{+-} - D_{32}^{+-}) - 2\Re(D_{31}^{+-} - D_{13}^{+-}) + 2\Im(D_{21}^{++} - D_{21}^{--}), \quad (43)$$

- vector densities

$$s_1 = 2\Re D_{00}^{+-}, \quad (44a)$$

$$s_2 = -2\Im D_{00}^{+-}, \quad (44b)$$

$$s_3 = D_{00}^{++} - D_{00}^{--}, \quad (44c)$$

$$T_1 = 2\Re \sum_{\mu} D_{\mu\mu}^{+-}, \quad (45a)$$

$$T_2 = -2\Im \sum_{\mu} D_{\mu\mu}^{+-}, \quad (45b)$$

$$T_3 = \sum_{\mu} (D_{\mu\mu}^{++} - D_{\mu\mu}^{--}), \quad (45c)$$

$$\Delta s_1 = 2\Re(L^{+-} + L^{-+}) + 2T_1, \quad (46a)$$

$$\Delta s_2 = 2\Im(L^{+-} - L^{-+}) + 2T_2, \quad (46b)$$

$$\Delta s_3 = 2(L^{++} - L^{--}) + 2T_3, \quad (46c)$$

$$\nabla \rho_{\mu} = 2\Re(D_{\mu 0}^{++} + D_{\mu 0}^{--}), \quad (47)$$

$$j_{\mu} = \Im(D_{\mu 0}^{++} + D_{\mu 0}^{--}), \quad (48)$$

$$(\nabla \times \mathbf{s})_1 = 2\Re(D_{20}^{++} - D_{20}^{--}) + 2\Im(D_{30}^{+-} + D_{03}^{+-}), \quad (49a)$$

$$(\nabla \times \mathbf{s})_2 = 2\Re(D_{30}^{+-} + D_{03}^{+-}) - 2\Re(D_{10}^{++} - D_{10}^{--}), \quad (49b)$$

$$(\nabla \times \mathbf{s})_3 = -2\Im(D_{10}^{+-} + D_{01}^{+-}) - 2\Re(D_{20}^{+-} + D_{02}^{+-}), \quad (49c)$$

$$(\nabla \times \mathbf{j})_1 = 2\Im \left( D_{32}^{++} + D_{32}^{--} \right), \quad (50a)$$

$$(\nabla \times \mathbf{j})_2 = -2\Im \left( D_{31}^{++} + D_{31}^{--} \right), \quad (50b)$$

$$(\nabla \times \mathbf{j})_3 = 2\Im \left( D_{21}^{++} + D_{21}^{--} \right), \quad (50c)$$

- tensor density

$$J_{\mu 1} = \Im \left( D_{\mu 0}^{+-} - D_{0\mu}^{+-} \right), \quad (51a)$$

$$J_{\mu 2} = \Re \left( D_{\mu 0}^{+-} - D_{0\mu}^{+-} \right), \quad (51b)$$

$$J_{\mu 3} = \Im \left( D_{\mu 0}^{++} - D_{\mu 0}^{--} \right). \quad (51c)$$

### 3 Self-consistent symmetries

#### 3.1 Simplex

The reader is referred to Ref. [31] for a detailed discussion of various possible choices of conserved symmetries and of the implications thereof. In the present version of the code HFODD we assume  $x$ - $z$  plane as *a priori* the only symmetry plane of the HF states. Such an assumption has been dictated exclusively by the fact that the CPU time for a typical run is markedly lower when symmetries are assumed. However, in physical applications one usually requires that all symmetries are determined by the physical system itself as a result of the self-consistency condition and not by a pre-supposition. We find that the assumption of a single symmetry plane provides an acceptable compromise between the above conflicting criteria.

As a consequence of the above assumption, the  $y$ -simplex operator, defined by

$$\hat{S}_y = \hat{P} \exp \left( -i\pi \hat{J}_y \right), \quad (52)$$

where  $\hat{P}$  is the parity operator, commutes with the single-particle Routhian operators (26), i.e.,

$$[h'_n, \hat{S}_y] = [h'_p, \hat{S}_y] = 0, \quad (53)$$

and that the many-body wave function  $|\Psi\rangle$  is an eigenstate of  $\hat{S}_y$ :

$$\hat{S}_y |\Psi\rangle = S |\Psi\rangle. \quad (54)$$

There are some technical advantages of choosing of the  $y$ -simplex as the conserved symmetry. One of them is related to the convenient phase relations which are discussed below; another one consists in the fact that the average values of multipole moments:

$$Q_{\lambda\mu} = \langle \hat{Q}_{\lambda\mu} \rangle \equiv \langle \Psi | \hat{Q}_{\lambda\mu} | \Psi \rangle \quad (55)$$

are real, i.e.,

$$Q_{\lambda\mu}^* = Q_{\lambda\mu}. \quad (56)$$

This property results from combining the standard time-invariance condition [32],

$$\hat{Q}_{\lambda\mu}^* = (-1)^\mu \hat{Q}_{\lambda,-\mu}, \quad (57)$$

with the transformation law under the operation of the  $y$ -simplex:

$$\hat{S}_y^\dagger \hat{Q}_{\lambda\mu} \hat{S}_y = (-1)^\mu \hat{Q}_{\lambda,-\mu}. \quad (58)$$

Equations (56)–(57) allow to consider only (real) multipole moments with non-negative magnetic components,  $\mu \geq 0$ . Apart from a restriction to real values, all multipole moments can be non-zero. In particular, deformations corresponding to four magnetic components,  $\mu=0, 1, 2$ , and  $3$ , of the octupole moment can be simultaneously present.

The choice of the  $y$ -simplex as a conserved symmetry requires that the nuclear rotation (cranking) takes place around the  $y$  axis. In the following we refer to the  $y$ -simplex as the simplex, and keep in mind that this axis corresponds to the rotation axis.

Because

$$\hat{S}_y^2 = (-1)^A, \quad (59)$$

the simplex has four eigenvalues:  $S=\pm 1$  and  $S=\pm i$  for even and odd numbers of particles, respectively. Due to the commutation relations (53), the single-particle Routhians do not have non-zero matrix elements between states belonging to different eigenvalues of  $\hat{S}_y$ . The equations for the single-particle eigenvalues can, therefore, be solved separately for both values of the single-particle simplex  $s=\pm i$ , and the single-particle wave functions  $\psi_{i,\alpha}(\mathbf{r}\sigma)$  are labeled by these values of the simplex, i.e.,

$$\hat{S}_y \psi_{i,\alpha}(\mathbf{r}\sigma) = s_i \psi_{i,\alpha}(\mathbf{r}\sigma). \quad (60)$$

In the above relation we do not introduce  $s_i$  as an extra label of the wave function since, according to our convention, all quantum numbers characterizing the single-particle states are contained within the index  $i$ . Throughout the code, input data, and output files we associate the sign “+” with the eigenvalue  $s=+i$  of the simplex operator  $\hat{S}_y$ , and the sign “−” with the eigenvalue  $s=-i$ .

### 3.2 Time-reversal

The code HFODD solves the HF equations with or without the time-reversal symmetry imposed, depending on the value of the input parameter IROTAT (see II, Sec. 3.3). However, the antiunitary time-reversal operator  $\hat{T}$

$$\hat{T} = -i\sigma_y \hat{K}_0, \quad \hat{T}^2 = (-1)^A, \quad (61)$$

where  $\hat{K}_0$  is the complex conjugation in coordinate space, is used throughout to establish the phases of the HO-basis simplex eigenstates, Sec. 4.1.

Since the time-reversal operator commutes with the simplex operator,

$$\hat{T} \hat{S}_y = \hat{S}_y \hat{T} \quad (62)$$

the time-reversed single-particle states belong to opposite simplex eigenvalues. (Recall that the antilinear time-reversal operator changes the sign of the imaginary simplex eigenvalue.) Therefore, only matrix elements for one of the eigenvalues, say  $s=+i$ , have to be

evaluated, while those for  $s=-i$  can be obtained by the time-reversal. One has only to keep track of the time-even and time-odd terms in the Routhians. When both kinds of terms are non-zero, as is for the case of rotation, the Routhians for both  $s$  eigenvalues have to be diagonalized. However, when the time-reversal symmetry is present (no rotation), only one diagonalization is sufficient.

### 3.3 Parity and signature

The code HFODD solves the HF equations with or without the parity symmetry imposed, depending on the value of the parameter `ISIGNY` chosen in the input data (see II, Sec. 3.3). Since the simplex  $\hat{S}_y$ , Eq. (52), is in the present implementation always a conserved symmetry, the case of conserved parity is in fact realized by requiring that the  $y$ -signature (signature for short), defined by

$$\hat{R}_y = \exp(-i\pi\hat{J}_y), \quad (63)$$

is a conserved symmetry. Then, the HF single-particle states are in addition labeled by the signature eigenvalues,  $r=\pm i$ ,

$$\hat{R}_y\psi_{i,\alpha}(\mathbf{r}\sigma) = r_i\psi_{i,\alpha}(\mathbf{r}\sigma), \quad (64)$$

while the simplex is a product of parity  $\pi$  and signature  $r$ ,  $s=\pi r$ , or equivalently the parity is a product of simplex and signature,  $\pi=sr^*$ . As before, the signature quantum number  $r_i$  is not attached explicitly as a label of the wave function. The  $s=+i$  block splits into two parity-signature blocks  $(\pi,r)=(+1,+i)$  and  $(-1,-i)$ , and similarly the  $s=-i$  block splits into  $(-1,+i)$  and  $(+1,-i)$ . These four blocks can be diagonalized separately. Throughout the code, input data, and output files we associate the sign “+” with the eigenvalue  $r=+i$  of the signature operator  $\hat{R}_y$ , and the sign “-” with the eigenvalue  $r=-i$ .

In the case of conserved parity and signature, the multipole moments  $Q_{\lambda\mu}$  vanish for odd values of  $\lambda$ , which is a consequence of the transformation law for multipole moments:

$$\hat{P}^\dagger \hat{Q}_{\lambda\mu} \hat{P} = (-1)^\lambda \hat{Q}_{\lambda\mu}. \quad (65)$$

### 3.4 T-simplexes

In addition to the two important cases of either the simplex  $\hat{S}_y$  alone appearing as a conserved quantity, or of the parity and signature  $\hat{R}_y$  being conserved, one may have two other cases of conserved symmetries. These symmetries cannot give any new quantum numbers simultaneously with the simplex  $s$ , because none of the other simplexes,  $\hat{S}_x$  and  $\hat{S}_z$ , or signatures,  $\hat{R}_x$  or  $\hat{R}_z$ , commutes with  $\hat{S}_y$ . However, we may still have conserved antilinear operators, which do not provide quantum numbers, but restrict spatial properties of solutions. The code HFODD can treat two such a symmetries [31], the  $x$ -simplex<sup>T</sup> and the  $z$ -simplex<sup>T</sup>,

$$\hat{S}_x^T = \hat{T}\hat{P}\exp(-i\pi\hat{J}_x), \quad (\hat{S}_x^T)^2 = 1, \quad (66a)$$

$$\hat{S}_z^T = \hat{T}\hat{P}\exp(-i\pi\hat{J}_z), \quad (\hat{S}_z^T)^2 = 1. \quad (66b)$$

These symmetries are requested by activating in the input data (see II, Sec. 3.3) the options **ISIMTX** and **ISIMTZ**, respectively. The product of these two symmetries equals to the  $y$ -signature,

$$\hat{S}_x^T \hat{S}_z^T = \hat{R}_y. \quad (67)$$

Therefore, if the Hamiltonian commutes with both of them, the signature (and hence parity) must also be conserved.

The two  $T$ -simplexes transform the multipole moments in the following way:

$$(\hat{S}_x^T)^\dagger \hat{Q}_{\lambda\mu} \hat{S}_x^T = (-1)^\mu \hat{Q}_{\lambda\mu}, \quad (68a)$$

$$(\hat{S}_z^T)^\dagger \hat{Q}_{\lambda\mu} \hat{S}_z^T = (-1)^\lambda \hat{Q}_{\lambda,-\mu}, \quad (68b)$$

which combined with the time-reversal and  $y$ -simplex transformation laws (57) and (58) gives, respectively, the following properties of multipole moments:

$$Q_{\lambda\mu} = (-1)^\mu Q_{\lambda\mu}, \quad (69a)$$

$$Q_{\lambda\mu} = (-1)^{\lambda+\mu} Q_{\lambda\mu}. \quad (69b)$$

Therefore, commutation of  $\hat{S}_x^T$  with the Hamiltonian enforces the vanishing of all odd magnetic components of all multipole moments. Nevertheless, with broken parity, the even magnetic components of odd multipoles, like  $Q_{30}$  and  $Q_{32}$ , can be nonzero. On the other hand, conservation of  $\hat{S}_z^T$  enforces the vanishing of odd magnetic components of even multipoles, and the vanishing of even magnetic components of odd multipoles. Therefore, with broken parity, the moments  $Q_{31}$  and  $Q_{33}$  can be nonzero. Of course, conservation of both  $T$ -simplexes leaves nonzero only even magnetic components of even multipoles. Table 1 summarizes the properties of multipole moments under different symmetry conditions. One should note that the broken parity may lead to the system which has the center of mass shifted from the origin,  $Q_{10} \neq 0$  and/or  $Q_{11} \neq 0$ , while for the both  $T$ -simplexes broken it may in addition lead to a shape which is not in the principal axes of the quadrupole tensor,  $Q_{21} \neq 0$ . In order to avoid physically meaningless “deformations” which in fact correspond to a shift or to a rotation of the whole system, one has to use suitable constraints, see Sec. 2.3 and II – Sec. 3.7, to enforce conditions  $Q_{10}=Q_{11}=Q_{21}=0$  in cases where the non-zero values are, in principle, allowed by broken symmetries.

Condition (67) means that there exist a possibility [31] of breaking both antilinear symmetries,  $\hat{S}_x^T$  and  $\hat{S}_z^T$ , and still conserving the signature (and hence parity). Such a possibility is, however, excluded from the present version of the code. This is so because, it would have corresponded to a state with vanishing octupole moments, and nevertheless non-zero moments  $Q_{41}$  and  $Q_{43}$  present in the principal-axes reference frame ( $Q_{21}=0$ ). The shapes of that type are very exotic indeed, cf. Ref. [33], and probably should be studied after an investigation of those corresponding to non-zero moments  $Q_{41}$  and  $Q_{43}$  induced by the non-zero octupole deformation. The latter possibility is allowed in the code HFODD.

## 4 Cartesian harmonic oscillator basis

The code HFODD solves the HF equations by expanding the single-particle wave functions  $\psi_i(\mathbf{r}\sigma)$  onto the deformed HO wave functions  $\psi_{n_x n_y n_z, s_z}(\mathbf{r}\sigma)$  in the Cartesian coordinates,

i.e.,

$$\psi_i(\mathbf{r}\sigma) = \sum_{n_x=0}^{N_x} \sum_{n_y=0}^{N_y} \sum_{n_z=0}^{N_z} \sum_{s_z=-\frac{1}{2}, \frac{1}{2}} A_i^{n_x n_y n_z s_z} \psi_{n_x n_y n_z s_z}(\mathbf{r}\sigma). \quad (70)$$

Here  $N_x$ ,  $N_y$ , and  $N_z$  are the maximum numbers of the HO quanta corresponding to the three Cartesian directions. However, as discussed in Sec. 2 of II, the sums over  $n_x$ ,  $n_y$ , and  $n_z$  are performed over the grid of points which form a pyramid rather than a cube.

The HO wave functions have the standard form

$$\psi_{n_x n_y n_z s_z}(\mathbf{r}\sigma) = \psi_{n_x}(x) \psi_{n_y}(y) \psi_{n_z}(z) \delta_{s_z \sigma}, \quad (71)$$

where

$$\psi_{n_\mu}(x_\mu) = b_\mu^{\frac{1}{2}} H_{n_\mu}^{(0)}(\xi_\mu) e^{-\frac{1}{2}\xi_\mu^2}, \quad (72)$$

and  $\xi_\mu = b_\mu x_\mu$  are dimensionless variables scaled by the oscillator constants

$$b_\mu = \sqrt{m\omega_\mu/\hbar}. \quad (73)$$

Polynomials  $H_n^{(0)}(\xi)$  are proportional to the standard Hermite orthogonal polynomials  $H_n(\xi)$  [34],

$$H_n^{(0)}(\xi) = \left(\sqrt{\pi} 2^n n!\right)^{-\frac{1}{2}} H_n(\xi), \quad (74)$$

and normalized as

$$\int_{-\infty}^{\infty} d\xi H_n^{(0)}(\xi) H_{n'}^{(0)}(\xi) e^{-\xi^2} = \delta_{nn'}. \quad (75)$$

When convenient, we also use the standard bra-ket notation:

$$|n_x n_y n_z, s_z\rangle \equiv \psi_{n_x n_y n_z s_z}(\mathbf{r}\sigma). \quad (76)$$

#### 4.1 Simplex basis

The  $y$ -simplex symmetry operator (52) transforms the HO states (76) in the following way

$$\hat{S}_y |n_x n_y n_z, s_z\rangle = (-1)^{n_y + \frac{1}{2} - s_z} |n_x n_y n_z, -s_z\rangle. \quad (77)$$

Since in the present implementation of the code HFODD, the simplex symmetry is always assumed, it is convenient to use the HO basis composed of states which belong to a given simplex, i.e.,

$$|n_x n_y n_z, s=+i\rangle = \frac{1}{\sqrt{2}} \left( i^{n_y} |n_x n_y n_z, \frac{1}{2}\rangle - i^{-n_y+1} |n_x n_y n_z, -\frac{1}{2}\rangle \right), \quad (78a)$$

$$|n_x n_y n_z, s=-i\rangle = \frac{1}{\sqrt{2}} \left( -i^{n_y+1} |n_x n_y n_z, \frac{1}{2}\rangle + i^{-n_y} |n_x n_y n_z, -\frac{1}{2}\rangle \right), \quad (78b)$$

for which

$$\hat{S}_y |n_x n_y n_z, s=\pm i\rangle = (\pm i) |n_x n_y n_z, s=\pm i\rangle. \quad (79)$$

Since the HO wave functions are real, the time-reversal operator (61) transforms them in the following way

$$\hat{T} |n_x n_y n_z, s_z\rangle = (-1)^{\frac{1}{2} - s_z} |n_x n_y n_z, -s_z\rangle \quad (80)$$

The relative phases of states (78a) and (78b) have been chosen in such a way that the time reversal simply flips the simplex:

$$\hat{T}|n_x n_y n_z, s=\pm i\rangle = \pm |n_x n_y n_z, s=\mp i\rangle. \quad (81)$$

Having the relative phases established, we may still arbitrarily chose the absolute phases of, say, the  $s=+i$  simplex eigenstates. The choice in Eq. (78a) is made by considering the antiunitary operator  $\hat{K}$

$$\hat{K} = \hat{T}i\sigma_z, \quad \hat{K}^2 = 1. \quad (82)$$

This operator does not act on the space coordinates and therefore conserves quantum numbers  $n_x n_y n_z$ . Since it is an antilinear operator with the square equal to one, the phases in the spin space can always be chosen [35] in such a way that all the basis states are its eigenstates with the eigenvalues being equal to 1. Since  $\hat{K}$  commutes with  $\hat{T}$ , such a choice of phase convention made in (78a) applies in fact to both simplexes, i.e.,

$$\hat{K}|n_x n_y n_z, s=\pm i\rangle = |n_x n_y n_z, s=\pm i\rangle. \quad (83)$$

One should stress that  $\hat{K}$  is not a conserved symmetry, and therefore the HF single-particle states do not have any particular symmetry with respect to this operator.

## 4.2 Matrix elements in the simplex basis

The properties of the operator  $\hat{K}$  and the resulting phase properties allow to simplify the form the single-particle potentials (27) when evaluated between the simplex eigenstates. Indeed, for such a choice various terms in these potentials have matrix elements which are either real or imaginary, but not complex. As can be easily checked, in the *time-even* potentials the spin-independent terms and the terms proportional to  $\sigma_z$  are real, while the terms proportional to  $\sigma_x$  and  $\sigma_y$  are imaginary, whereas, in the *time-odd* potentials the spin-independent terms and the terms proportional to  $\sigma_z$  are imaginary, while the terms proportional to  $\sigma_x$  and  $\sigma_y$  are real. As already mentioned, the operator  $\hat{K}$  is not a conserved symmetry of the Routhians, the HF wave functions do not have any specific  $\hat{K}$  symmetry and are complex.

Let  $\hat{O}$  denote an arbitrary operator acting only in the space coordinates (independent of spin) and let  $|n_x n_y n_z\rangle$  denote pure HO states (no spin component). Then we may summarize the properties of matrix elements in the simplex basis in the following way:

$$\langle n_x n_y n_z, s=+i | \hat{O} \sigma_0 | n'_x n'_y n'_z, s=+i \rangle = \langle n_x n_y n_z | \hat{O} | n'_x n'_y n'_z \rangle F(n_y - n'_y), \quad (84a)$$

$$\langle n_x n_y n_z, s=+i | \hat{O} \sigma_x | n'_x n'_y n'_z, s=+i \rangle = \langle n_x n_y n_z | \hat{O} | n'_x n'_y n'_z \rangle F(n_y + n'_y + 1), \quad (84b)$$

$$\langle n_x n_y n_z, s=+i | \hat{O} \sigma_y | n'_x n'_y n'_z, s=+i \rangle = \langle n_x n_y n_z | \hat{O} | n'_x n'_y n'_z \rangle F(n_y + n'_y + 2), \quad (84c)$$

$$\langle n_x n_y n_z, s=+i | \hat{O} \sigma_z | n'_x n'_y n'_z, s=+i \rangle = \langle n_x n_y n_z | \hat{O} | n'_x n'_y n'_z \rangle i F(n_y - n'_y + 1), \quad (84d)$$

where the factors  $F(n)$  are defined as

$$F(n) = \begin{cases} (-1)^{\frac{n}{2}} & \text{for } n \text{ even,} \\ 0 & \text{for } n \text{ odd.} \end{cases} \quad (85)$$



These properties allow omitting the calculation of matrix elements for which  $F=0$ . As mentioned in Sec. 3.2, the matrix elements corresponding to  $s=-i$  need not be explicitly calculated.

### 4.3 Matrix elements in the coordinate space

For the Skyrme interaction, the Routhian operators (26) are differential operators composed of terms up to the second-order derivatives. Therefore, the spatial matrix elements of the type  $\langle n_x n_y n_z | \hat{O} | n'_x n'_y n'_z \rangle$  can be calculated by using differential formulas for the HO wave functions (72), i.e.,

$$\frac{d}{dx_\mu} \psi_{n_\mu}(x_\mu) = b_\mu^{\frac{3}{2}} H_{n_\mu}^{(1)}(\xi_\mu) e^{-\frac{1}{2}\xi_\mu^2}, \quad (86a)$$

$$\frac{d^2}{dx_\mu^2} \psi_{n_\mu}(x_\mu) = b_\mu^{\frac{5}{2}} H_{n_\mu}^{(2)}(\xi_\mu) e^{-\frac{1}{2}\xi_\mu^2}, \quad (86b)$$

where  $H_n^{(1)}(\xi)$  and  $H_n^{(2)}(\xi)$  are the  $(n+1)$ - and  $(n+2)$ -order polynomials of  $\xi$  defined by

$$H_n^{(1)}(\xi) = 2n H_{n-1}^{(0)}(\xi) - \xi H_n^{(0)}(\xi), \quad (87a)$$

$$H_n^{(2)}(\xi) = (\xi^2 - 2n - 1) H_n^{(0)}(\xi). \quad (87b)$$

Matrix elements of all types of differential operators (up to the second order) can therefore be expressed through the expansion coefficients  $C_{nn'}^k(dd')$ ,

$$H_n^{(d)}(\xi) H_{n'}^{(d')}(\xi) = \sum_{k=0}^{n+n'+d+d'} C_{nn'}^k(dd') H_k^{(0)}(\xi), \quad (88)$$

with  $0 \leq d+d' \leq 2$ , and through the integrals involving the polynomials  $H_k^{(0)}(\xi)$  only. Coefficients  $C_{nn'}^k(dd')$  can be in principle calculated recursively or explicitly [15], however, a method which is simpler and less prone to programming errors has been used in the code HFODD, namely, they are calculated numerically with the machine precision by employing the orthogonality relations (75) of Hermite polynomials and the Gauss-Hermite quadratures. From now on, we consider explicitly only those terms which do not contain derivatives, while all derivative terms can be treated analogously by using conditions (88) for  $d, d' > 0$ .

Concentrating on terms without derivatives, the matrix elements of an arbitrary function  $O(x, y, z)$  can be calculated as

$$\langle n_x n_y n_z | \hat{O} | n'_x n'_y n'_z \rangle = \sum_{k_x} C_{n_x n'_x}^{k_x}(00) \sum_{k_y} C_{n_y n'_y}^{k_y}(00) \sum_{k_z} C_{n_z n'_z}^{k_z}(00) O_{k_x k_y k_z}, \quad (89)$$

where

$$O_{k_x k_y k_z} = \int d\xi_x d\xi_y d\xi_z O\left(\frac{\xi_x}{b_x}, \frac{\xi_y}{b_y}, \frac{\xi_z}{b_z}\right) H_{k_x}^{(0)}(\xi_x) H_{k_y}^{(0)}(\xi_y) H_{k_z}^{(0)}(\xi_z) e^{-\xi_x^2 - \xi_y^2 - \xi_z^2}. \quad (90)$$

Integrals (90) are calculated by the standard Gauss-Hermite quadratures [34]. These integrals can be calculated *exactly* by noticing that for the Skyrme interaction the functions  $O(x, y, z)$  are linear combinations [see Eqs. (29)] of densities (39), which in turn are quadratic in the HO wave functions and their derivatives. Therefore, all<sup>3</sup> integrated functions  $O(x, y, z)$  have a form of polynomials  $W(x, y, z)$  multiplied by the typical HO Gaussian factors, i.e.,

$$O(x, y, z) = W(x, y, z)e^{-\xi_x^2 - \xi_y^2 - \xi_z^2}, \quad (91)$$

for  $\xi_\mu = b_\mu x_\mu$ , cf. Eq. (73). By including the Gaussian factors explicitly in the Gauss-Hermite quadratures one can calculate the integrals of the remaining polynomials exactly, i.e.,

$$\begin{aligned} O_{k_x k_y k_z} &= \int d\xi_x d\xi_y d\xi_z W\left(\frac{\xi_x}{b_x}, \frac{\xi_y}{b_y}, \frac{\xi_z}{b_z}\right) H_{k_x}^{(0)}(\xi_x) H_{k_y}^{(0)}(\xi_y) H_{k_z}^{(0)}(\xi_z) e^{-2\xi_x^2 - 2\xi_y^2 - 2\xi_z^2} \\ &= \frac{1}{\sqrt{8}} \int d\eta_x d\eta_y d\eta_z W\left(\frac{\eta_x}{\sqrt{2}b_x}, \frac{\eta_y}{\sqrt{2}b_y}, \frac{\eta_z}{\sqrt{2}b_z}\right) H_{k_x}^{(0)}\left(\frac{\eta_x}{\sqrt{2}}\right) H_{k_y}^{(0)}\left(\frac{\eta_y}{\sqrt{2}}\right) H_{k_z}^{(0)}\left(\frac{\eta_z}{\sqrt{2}}\right) e^{-\eta_x^2 - \eta_y^2 - \eta_z^2} \\ &= \sum_{l_x=1}^{L_x} G_{k_x}^{l_x} \sum_{l_y=1}^{L_y} G_{k_y}^{l_y} \sum_{l_z=1}^{L_z} G_{k_z}^{l_z} W\left(\frac{\eta_{l_x}}{\sqrt{2}b_x}, \frac{\eta_{l_y}}{\sqrt{2}b_y}, \frac{\eta_{l_z}}{\sqrt{2}b_z}\right). \end{aligned} \quad (92)$$

In the final formula,  $\eta_l$  are the standard Gauss-Hermite nodes [34] and the corresponding weights  $w_l$  are included in the matrices  $G_k^l$ , i.e.,

$$G_k^l = \frac{w_l}{\sqrt{2}} H_k^{(0)}\left(\frac{\eta_l}{\sqrt{2}}\right). \quad (93)$$

The orders  $L_x$ ,  $L_y$ , and  $L_z$  of the Gauss-Hermite quadratures can be estimated from the maximum numbers of HO quanta included in the basis, Eq. (70). These quadratures give exact results, also for terms depending on derivatives, for

$$L_\mu = 2N_\mu + 2, \quad (94)$$

or larger.

It turns out that the CPU time required to perform the summations in Eq. (92) is very small compared to other parts of the code. It is so provided the order of summations is as indicated in the formula, whence at most four-fold nested loops are required. A much larger effort is required to perform the summations in Eq. (89), where, even with the indicated order of sums, the seven-fold nested loops are necessary. Even if, in practice, the dimensions of these loops are rather small, this requires a substantial numerical effort. This is also the part of the code which is least amenable to vectorization. Such considerations indicate that the use of the Gauss-Hermite orders (94) ensuring exact integration is fully justified, even if these can be quite large for large numbers of HO quanta, and are certainly much larger than those usually used by other authors and codes.

From the presented analysis it is clear that the summations of the HF densities (39) have to be performed only at the spatial points which are defined by the Gauss-Hermite integration. Moreover, the same derivatives of HO wave functions as in Eqs. (86) can be

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<sup>3</sup>Except from the terms resulting from the density dependence (30), and from the exchange Coulomb terms (19). The direct Coulomb terms are treated separately in Sec. 5.

used to calculate the derivative densities in Eq. (39). The spatial symmetries discussed in Sec. 3 are employed to reduce the number of points in space where the densities have to be summed up, i.e., for three, two, or one symmetry planes only 1/8, 1/4, or, 1/2 points, respectively, are used. Table 2 summarizes the symmetries of different HF densities with respect to the  $y$ - $z$ ,  $x$ - $z$ , or  $x$ - $y$  plane [31]. These three symmetry planes are independent of one another and appear for the conserved symmetries  $\hat{S}_x^T$ ,  $\hat{S}_y$ , and  $\hat{S}_z^T$ , respectively, although, as discussed above, not leading to the conserved quantum numbers (except if the parity is implied).

## 5 Direct Coulomb potential

Direct Coulomb potential is given by three-dimensional integral (18) and therefore differs from all the Skyrme mean-field potentials (29) which are simple linear combinations of densities. Various methods of calculating this potential are used in the existing HF codes. A direct integration of the Poisson equation can be performed in the one-dimensional calculations restricted to the spherical symmetry. In two-dimensional calculations performed for axially deformed nuclei such an integration is also possible [36]. In three dimensions one may either solve the Poisson equation by using the conjugate gradient method [37] or replace the Coulomb interaction by an integral over Gaussian interactions [15, 38]. The latter method is very convenient for the Gogny interaction for which the matrix elements of Gaussians have to be anyhow calculated.

In the code HFODD we have implemented the method based on using the Coulomb Green function [39], which is particularly well suited for calculations employing the Cartesian HO basis. This is so because the Coulomb potential (18) is then, in fact, not explicitly required; it is enough to calculate its HO-basis matrix elements.

The direct Coulomb potential (18) can be expressed through the Dirichlet Green function  $G_D(\mathbf{r}, \mathbf{r}')$  in the following way [39]

$$U^{\text{Coul}}(\mathbf{r}) = e^2 \int_V d^3\mathbf{r}' G_D(\mathbf{r}, \mathbf{r}') \rho_p(\mathbf{r}') - \frac{1}{4\pi} \oint_S d^2s' \frac{\partial G_D(\mathbf{r}, \mathbf{r}')}{\partial n'} U^{\text{Coul}}(\mathbf{r}'). \quad (95)$$

The first term is the volume integral over an arbitrary closed volume, while the second integral is performed over the surface of this volume. The Coulomb potential has to be known on the surface. The Dirichlet Green function fulfills the Poisson equation for a point charge and vanishes at the surface. In the surface term, the normal derivative is calculated with respect to the outward direction perpendicular to the surface.

In the present application it is convenient to use in (95) the volume in the form of the parallelepiped

$$\begin{aligned} -D_x &\leq x \leq D_x, \\ -D_y &\leq y \leq D_y, \\ -D_z &\leq z \leq D_z. \end{aligned} \quad (96)$$

Then, the required Green function can be expressed in a separable form as

$$G_D(\mathbf{r}, \mathbf{r}') = \frac{4\pi}{D_x D_y D_z} \sum_{j_x j_y j_z} \frac{f(J_x x) f(J_y y) f(J_z z) f(J_x x') f(J_y y') f(J_z z')}{J_x^2 + J_y^2 + J_z^2}, \quad (97)$$

where the functions  $f$  equal to sine or cosine ensuring the Dirichlet boundary conditions:

$$f(J_\mu x_\mu) = \begin{cases} \cos(J_\mu x_\mu) & \text{for } j_\mu \text{ even,} \\ \sin(J_\mu x_\mu) & \text{for } j_\mu \text{ odd,} \end{cases} \quad (98)$$

and

$$J_\mu = \frac{(j_\mu + 1)\pi}{2D_\mu}. \quad (99)$$

In expression (97), the sums over  $j_x$ ,  $j_y$ , and  $j_z$  are performed over all non-negative integer values. In practice, these sums have to be restricted to finite ranges. In the code HFODD we use the summation bounds

$$0 \leq j_x, j_y, j_z \leq N^{\text{Coul}}, \quad (100)$$

and  $N^{\text{Coul}}$  can be chosen based on the following considerations: It is clear that when using the Green function for the calculation of the Coulomb potential one must effectively perform the Fourier transform of the proton density. Therefore, the corresponding wave vectors  $J_\mu$  have to cover the region of momenta for which the proton momentum density distribution is large. This distribution is localized in the momentum space, i.e., does not extend to very large momenta; therefore, the sums can be terminated for indices  $j_\mu$  giving suitable large fixed values of  $J_\mu$ . The value of  $N^{\text{Coul}}$  depends, therefore, linearly on the steps in the momentum space given by  $\pi/(2D_\mu)$ , and hence inversely on the dimensions  $D_\mu$ . Therefore, we are interested in working with appropriately small sizes  $D_\mu$  of the parallelepiped.

On the other hand, one has also to know the values of the Coulomb potential on the six faces of the parallelepiped. Suppose these faces are located far enough, where the proton density is already very small. Then the Coulomb potential on these faces can be very well approximated by the standard multipole expansion [39]

$$U^{\text{Coul}}(\mathbf{r}) = \sum_{\lambda\mu} \frac{4\pi e^2}{(2\lambda + 1)r^{2\lambda+1}} Q_{\lambda\mu}^p r^\lambda Y_{\lambda\mu}(\theta, \phi). \quad (101)$$

For the validity and precision of the multipole expansion truncated to a few lowest values of  $\lambda$ , we are interested in working with appropriately large sizes  $D_\mu$  of the parallelepiped.

In practice it turns out that one can chose suitable dimensions of the parallelepiped so as to fulfill both requirements simultaneously. In the code HFODD the dimensions in three directions are chosen to be proportional to the corresponding oscillator lengths  $1/b_\mu$ , i.e.,

$$D_\mu = \frac{d}{\sqrt{2}b_\mu}, \quad (102)$$

where  $d$  is a dimensionless parameter defining the overall size of the parallelepiped. Based on the performed numerical tests, the recommended values are  $d=20$  and  $N^{\text{Coul}}=80$ , which for a heavy nucleus corresponds to the parallelepiped of about  $D_\mu \sim 30$  fm, and to the maximum momentum and the integration step in the Fourier transforms of about  $4 \text{ fm}^{-1}$  and  $0.05 \text{ fm}^{-1}$ , respectively. For the SD states in  $^{152}\text{Dy}$  the maximum contributions of the monopole, quadrupole, and hexadecapole terms to the Coulomb potential are at the

surface of the  $D_\mu \sim 30$  fm cube equal to about 3 MeV, 50 keV, and 1.5 keV, respectively. In the multipole expansion of Eq. (101) the multipoles above  $\lambda=4$  can therefore be safely neglected.

The calculation of the HO matrix elements of the Coulomb potential can now be very easily completed. First, we insert the multipole expansion (101) in the surface term in Eq. (95). All surface integrals can now be performed, because they amount to suitable Fourier transforms of the solid harmonics  $r^\lambda Y_{\lambda\mu}$  on the six faces of the parallelepiped. The values of proton multipole moments  $Q_{\lambda\mu}^p$  are anyhow routinely calculated for the determination of nuclear deformations.

Second, we use the fact that the proton density has the form of a polynomial multiplied by the HO Gaussian factor [cf. Eq. (91)],

$$\rho^p(x, y, z) = W_\rho^p(x, y, z) e^{-\xi_x^2 - \xi_y^2 - \xi_z^2}, \quad (103)$$

and this polynomial can be expressed *exactly* as a linear combination of Hermite polynomials,

$$W_\rho^p(x, y, z) = \sum_{k_x k_y k_z} \rho_{k_x k_y k_z}^p H_{k_x}^{(0)}(\sqrt{2}b_x x) H_{k_y}^{(0)}(\sqrt{2}b_y y) H_{k_z}^{(0)}(\sqrt{2}b_z z). \quad (104)$$

Here, for later convenience we have included the factors  $\sqrt{2}$  in the arguments of the normalized Hermite polynomials.

Coefficients  $\rho_{k_x k_y k_z}^p$  can be calculated (again exactly) by using the Gauss-Hermite quadratures of the order given by Eq. (94) in the formula analogous to (90). In fact, if we want to use the same Gauss-Hermite nodes as before, we have to employ the formula

$$\rho_{k_x k_y k_z}^p = \sum_{l_x=1}^{L_x} G_{k_x}^{l_x} \sum_{l_y=1}^{L_y} G_{k_y}^{l_y} \sum_{l_z=1}^{L_z} G_{k_z}^{l_z} W_\rho^p\left(\frac{\eta_{l_x}}{\sqrt{2}b_x}, \frac{\eta_{l_y}}{\sqrt{2}b_y}, \frac{\eta_{l_z}}{\sqrt{2}b_z}\right), \quad (105)$$

for

$$G_k^l = w_l H_k^{(0)}(\eta_l). \quad (106)$$

Third, we insert the proton density in the form of Eqs. (103) and (104) in the volume integral in Eq. (95). Then we see that the Fourier transform of proton density amounts to calculating the Fourier transforms of the HO oscillator wave functions. In practice, the dimensions of the parallelepiped are large enough to replace these transforms by the analytic results pertaining to integrations extended to infinity, i.e.,

$$\begin{aligned} B_k^j &= \int_{-d}^d d\eta f(\omega_j \eta) H_k^{(0)}(\eta) e^{-\frac{1}{2}\eta^2} \\ &\simeq \begin{cases} \sqrt{2\pi} H_k^{(0)}(\omega_j) e^{-\frac{1}{2}\omega_j^2} (-1)^{\left[\frac{k}{2}\right]} & \text{for } k+j \text{ even,} \\ 0 & \text{for } k+j \text{ odd,} \end{cases} \end{aligned} \quad (107)$$

where

$$\omega_j = \frac{(j+1)\pi}{2d}, \quad (108)$$

and  $\left[\frac{k}{2}\right]$  denotes the integer part. Due to the choice of parallelepiped dimensions adapted to the basis, Eq. (102), the factors  $B_k^j$  are the same for each Cartesian direction.

After these manipulations, the Coulomb potential, the volume and surface terms alike, are expressed as linear combinations of terms proportional to  $f(J_x x)f(J_y y)f(J_z z)$ . Instead of performing this sums, and calculating the Coulomb potential in spatial coordinates, one may rather directly calculate its HO-basis matrix elements. This gives

$$U'_{k_x k_y k_z}{}^{\text{Coul}} = \frac{8e^2}{\pi d} \sum_{j_x} B_{k_x}^{j_x} \sum_{j_y} B_{k_y}^{j_y} \sum_{j_z} B_{k_z}^{j_z} \frac{V_{j_x j_y j_z} + \sum_{\lambda\mu} Q_{\lambda\mu}^p S_{j_x j_y j_z}^{\lambda\mu}}{b_x^2(j_x + 1)^2 + b_y^2(j_y + 1)^2 + b_z^2(j_z + 1)^2}, \quad (109)$$

where the volume term reads

$$V_{j_x j_y j_z} = \sum_{k_x} B_{k_x}^{j_x} \sum_{k_y} B_{k_y}^{j_y} \sum_{k_z} B_{k_z}^{j_z} \rho_{k_x k_y k_z}^p, \quad (110)$$

and the sums in Eq. (109) are restricted to the finite set of indices (100).

In Eq. (109) the surface term is a linear combination of proton multipole moments multiplied by fixed matrices  $S_{j_x j_y j_z}^{\lambda\mu}$ . These matrices are calculated only once by integrating solid harmonics on the faces of the parallelepiped. Finally, the Coulomb matrix elements are obtained from

$$\langle n_x n_y n_z | \hat{U}^{\text{Coul}} | n'_x n'_y n'_z \rangle = \sum_{k_x} C'^{k_x}_{n_x n'_x} \sum_{k_y} C'^{k_y}_{n_y n'_y} \sum_{k_z} C'^{k_z}_{n_z n'_z} U'_{k_x k_y k_z}{}^{\text{Coul}}, \quad (111)$$

where the new set of coefficients  $C'^{k}_{nn'}$  is required to accommodate the additional factor of  $\sqrt{2}$ , i.e.,

$$H_n^{(0)}(\xi) H_{n'}^{(0)}(\xi) = \sum_{k=0}^{n+n'} C'^{k}_{nn'} H_k^{(0)}(\sqrt{2}\xi). \quad (112)$$

Similarly as for other terms of Routhians, evaluation of sums in Eqs. (109) and (110) requires much less numerical effort than of those in Eq. (111).

The Green function method allows calculating the matrix elements of the Coulomb field directly from the matrix elements of the proton density. The summations involved require the numerical effort which is typical for other terms of the Skyrme interaction, in spite of the fact that the Coulomb interaction is not of zero-order. Performing the sums in the order indicated in Eqs. (109) and (110) never leads to more than four-fold nested loops over low-dimension indices.

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Table 1: Pattern of allowed non-zero values (denoted by X) of the expectation values of the multipole moment operators for four different cases of symmetries treated by the HFODD code.

Symmetry planes:	one, $x$ - $z$	two, $x$ - $z$ and $y$ - $z$	two, $x$ - $z$ and $x$ - $y$	three
Conserved:	$\hat{S}_y$	$\hat{S}_y$ and $\hat{S}_x^T$	$\hat{S}_y$ and $\hat{S}_z^T$	$\hat{S}_y$ , $\hat{S}_x^T$ , and $\hat{S}_z^T$
$Q_{10}$	X	X	0	0
$Q_{11}$	X	0	X	0
$Q_{20}$	X	X	X	X
$Q_{21}$	X	0	0	0
$Q_{22}$	X	X	X	X
$Q_{30}$	X	X	0	0
$Q_{31}$	X	0	X	0
$Q_{32}$	X	X	0	0
$Q_{33}$	X	0	X	0
$Q_{40}$	X	X	X	X
$Q_{41}$	X	0	0	0
$Q_{42}$	X	X	X	X
$Q_{43}$	X	0	0	0
$Q_{44}$	X	X	X	X

Table 2: Symmetries of HF densities with respect to the three symmetry planes appearing when one of the three different symmetries are conserved.

Conserved:	$\hat{S}_x^T$	$\hat{S}_y$	$\hat{S}_z^T$	Conserved:	$\hat{S}_x^T$	$\hat{S}_y$	$\hat{S}_z^T$
Plane:	$y$ - $z$	$x$ - $z$	$x$ - $y$	Plane:	$y$ - $z$	$x$ - $z$	$x$ - $y$
$\rho$	+	+	+	$\Delta\rho$	+	+	+
$\tau$	+	+	+	$\nabla \cdot \mathbf{J}$	+	+	+
$s_1$	-	-	+	$\nabla_1\rho$	-	+	+
$s_2$	+	+	+	$\nabla_2\rho$	+	-	+
$s_2$	+	-	-	$\nabla_3\rho$	+	+	-
$T_1$	-	-	+	$\Delta s_1$	-	-	+
$T_2$	+	+	+	$\Delta s_2$	+	+	+
$T_3$	+	-	-	$\Delta s_3$	+	-	-
$\dot{j}_1$	+	+	-	$(\nabla \times \mathbf{s})_1$	+	+	-
$\dot{j}_2$	-	-	-	$(\nabla \times \mathbf{s})_2$	-	-	-
$\dot{j}_3$	-	+	+	$(\nabla \times \mathbf{s})_3$	-	+	+
$J_{11}$	-	-	-	$(\nabla \times \mathbf{j})_1$	-	-	+
$J_{21}$	+	+	-	$(\nabla \times \mathbf{j})_2$	+	+	+
$J_{31}$	+	-	+	$(\nabla \times \mathbf{j})_3$	+	-	-
$J_{12}$	+	+	-				
$J_{22}$	-	-	-				
$J_{32}$	-	+	+				
$J_{13}$	+	-	+				
$J_{23}$	-	+	+				
$J_{33}$	-	-	-				